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MODEL LIQUID SELECTION BASED ON EXTREME VALUES OF LIQUID STATE PROPERTIES IN A FACTOR ANALYSIS

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Over 50 liquids with extreme values of liquid state properties were identified. The properties were hydrogen bond acceptor and donor strength, polarity, refractive index, density, and molecular weight. These model liquids can be selected for investigation of solvent-solute interactions to provide bold ANOVA experimental designs, orthogonal liquid experimental sets, and minimal co-correlation among experimental data.

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PREFACE

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1. INTRODUCTION

The purpose of this evaluation was to consider the application of appropriate experimental strategies to the investigation of the influence of liquid state properties (LSP) on the overall interactions of liquids.

The available calculated and measured properties of liquids have interactive effects on most dependent variables of interest. That is, (1) some degree of bond polarity must be present for a molecule to function as a proton acceptor; (2) dispersion forces usually increase with molecular weight (MW); (3) the solubility parameter contains dispersion, polar, and hydrogen bond (HB) effects, and so on. Measurement techniques or functional combinations of variables that totally isolate the specific intermolecular effect with the specific phenomenon are not yet available.

One approach is to employ factor analysis in the experimental design of liquid state investigations, whereby each of the candidate independent factor variables would be represented by an experiment at the two extreme levels and perhaps one mid-level value of the variable, e.g., MW, Vm, density, HB parameter(s) (HBP), polarity parameter(s), etc. Therefore, the purposes of this evaluation are (1) to analyze and select candidate model liquids at the extremes of LSP, (2) to consider the degree to which model liquids could be standardized for related investigations of LSP, and (3) to anticipate possible experimental and conceptual difficulties and the limitations of this strategy.

2. PROCEDURES

The specific incorporation of two extreme values in the experiment is termed a 'bold' design in statistical terminology. Current researchers intuitively recognize the need for inclusion of liquids with a wide range of properties in experimentation and the unavoidable interaction effects and co-correlation of independent variables. Attempts are made to regress and correlate a smooth sequence of LSP versus the independent response. However, most often, the intent and purpose of the investigation leads to a narrow range of LSPs. This cluster of points might well represent replicates of the midpoint in factor designs. The difference between a bold factor strategy and an immediate regression approach is the addition of at least two extreme LSP values. These extreme values might be incorporated in sequential experimentation either as an initial screening experiment or as values in an extensive correlation experiment.

An evaluation of the extreme values of LSP for the following parameters are itemized in Table 1: HBP, polar parameter (P), dispersion or nonpolar (D(NP)) parameters, refractive index (RI), density, and MW. In a sense, these parameters have already been modelled for regular solutions resulting in cohesion parameters. However, MW and density are retained rather than substitute Vm to maintain variables at their most fundamental values.

Table 1. Classification of Model Liquid Based on Values of Interaction Properties: Zero (Z), Co-Correlated in a Series (C), or Uncontrolled (U)

Properties		MW	NP	Density	Polar	Basicity	Acidity
Acidity	High	U	C	U	U	U	1.0
	Low	U	C	U	U	U	0.1
Basicity	High	U	U,C	U	U	1.0	Z
	Medium	U	U,C	U	U	0.3	Z
	Low	U	U,C	U	U	Z, 0.2	Z
Polar	High	U	C,U	U	1.05	Z,U	Z
	Medium	U	C,U	U	0.8-0.2	Z,U	Z
	Low	U	C,U	U	0.1	Z,U	Z
Density	High	C,U	C	2.5-3.5	Z	Z,U	Z
	Low	C,U	C	0.7	Z	Z,U	Z
Dispersion/ Nonpolar D(NP)	High	C	U,C	C	Z	Z	Z
	Low	C	U,C	C	Z	Z	Z
MW	High	2000-800	C	C	Z	Z,U	Z
	Low	100	C	C	Z	Z,U	Z

The opportunity might be provided to select model liquids that have an extreme value of some variable and a zero (Z) value for other variables. This simplification often slightly restricts the extreme range available because model liquids with a Z value for a parameter may not be available; in these cases, Z and non-Z extreme pairs are identified.

A related aspect requires a decision on selection of finite, non-Z values for the lower extremes for HBP and polarity. The finite values were selected for the following reasons:

a. The detection of the influence and sensitivity of the independent response to minimal values of HB or polarity is of importance.

b. The extreme values of other variables such as MW and density already provide adequate representation of model liquids with zero HBP and polarity.

Another criterion used was to identify monofunctional liquids whenever possible. In instances where difunctional liquids provide either favorable or more extreme properties, attempts are made to provide pairs of both monofunctional and difunctional liquids so the difunctional effect can be subtracted out.

Pragmatic considerations influenced the selection of model liquids in the following manner:

a. Moderate vapor pressures were favored for wide application as solvent media, reaction media, chromatography standards/carriers, etc. A BP criterion of 200 °C was emphasized.

b. Important commercial liquids, plasticizers, polymer repeat unit models, and widely used research solvents were favored when possible.

c. Model solutes were excluded and melting points (MP) below ambient temperature were required. In several cases, unique model liquids that melt very near ambient were identified, and addition of 'inert' impurities/cosolvents might be attempted to lower the melting point to exploit the unique properties of a model liquid.

Table 1 contains a matrix that classifies the values of the interactions in terms of the possibilities listed below:

a. If they are or can be held at Z values by choice of appropriate model liquids.

b. If the interactions are co-correlated (C) within a series of related liquids and model liquids in the series were identified.

c. If the other values of these variables are random (R) in that there were no selections that could be made to simplify the range of values for other properties of the liquid.

In Table 1, the columns and rows list each of the liquid state properties evaluated. The rows are subdivided into high, medium, and low rows for noting the approximate values selected for the LSP of interest and a further listing of the influence of the other LSP on the selection. Useful model liquid candidates were identified with a high range of MW at 2000-800 and low MW of about 100. The C series entry under density and nonpolar forces notes that densities and nonpolar forces varied directly with MW in one or more of the candidate model liquids. On the other hand, the model liquids selected possessed Z values for polarity and HB acidity, and some liquids were selected with Z and random values for HB basicity.

Data Sources

The linear solvation solute and solvent parameters were obtained from a merged and restructured dBase 4 version of Solubase from the Abraham Research Group.[1] Hansen cohesion parameters and hydrogen bond index (HBI) values were obtained from Barton.[2] Cohesion parameters were obtained from Hoy.[3] Dipole moment values were obtained from McClellan.[4] Physical properties were obtained from the Aldrich Computer-Search Database.[5]

3. RESULTS

3.1 Hydrogen Bond Parameters (HBPs).

Hydrogen bonding acceptor (HBA) liquids are listed in Table 2. Model liquids with high HBPs are listed followed by liquids with low, finite (non-zero) HBA substituents. The columns contain HBPs quantified by several different systems.

Table 2. Model Liquid Candidates with Extreme Values of HBA Parameters, (MPa) 1/2

Priority	Model Liquid	Basicity[1]	HBI[2]	Hansen[2]	Hoy[3]
	HIGH				
1	DMSO	0.76	7.7	10.2	nd*
2	Hexamethylphosphoramide	1.05	nd	11.3	nd
	LOW				
1	Methoxycycloheptatriene	0.2-0.4 est**	nd	5 est	6 est
2	Ethyl-2,3-dibromoproprionate (Aldrich E2,280-5)	0.2-0.3 est	3 est	nd	nd
	1,4,7,10,13-Pentaoxa-cyclopentadecane (15-Crown-5) with or w/o 18-Crown-6 eutetic) (Aldrich 18,883-2)	0.3-0.4	nd	9 est	nd

*nd = not determined
**est = estimate

The selection of aprotic dipolar (AD) liquids with extreme values of the beta HBA in the linear solvation energy relationship (LSER) system is limited. Hexamethylphosphoramide (HMPA) appears to be the lone high basicity liquid at a normalized value of 1.05. The next 25% of the scale contains few liquids until values below 0.8. Likewise, the lower range contains few liquids between 0 and 0.1, other than aromatics. Methoxycycloheptatrienes have low-to-moderate HBPs; substitution at different sites along the triene might also provide a range of polarities. These liquids are of importance because their rate of transport through skin is as rapid as that of dimethyl sulfoxide (DMSO), while their solvent parameters are quite different from DMSO, and their molecular cross-section is larger than that of DMSO.

A second group of liquids are halogenated esters (Table 2, Low, Priority 2). These esters have low HBP and rather high densities. An important model compound is a liquid crown ether. The general solute and solvent properties are of interest since they may indirectly influence the phase transfer catalytic activity of this class of compounds.

3.2 Hydrogen Bond Proton Acceptor/Donor Strength.

Proton acceptor/donor compounds are listed in Table 3. Certain haloalkanes with a proton activated by adjacent halogens are thought to function as weak proton donors. Weak proton-donating behavior is possible for specific alkynes and these are listed. Satisfactorily strong HBA liquids are known, and HFIP and DETA are listed. A more interesting and perhaps stronger HBA and/or donor liquid is listed as a bifluoride amine complex. This model liquid is related to Olah's reagent, without the excess pyridine. The other priority compounds are components of an important DoD cleaning solution (DS2, items 1 and 2).

Table 3. Model Liquid Candidates for Extreme Values of Proton-Donating Acidity

Priority	Model Liquid	Acidity[1]	HBI[2]	Hansen[2]	Hoy[3]
	HIGH				
1	Diethylenetriamine (DETA)	nd*	nd	14.3	14.7
2	Ethyleneglycolmonoethylether (Cellosolve)	0.7-0.9 est**	13	14.3	15.2
3	Hexafluoroisopropanol (HFIP)	1.96	nd	nd	nd
4	Bifluoride-Amine Liquid salts	high	nd	nd	nd
5	Dipropyleneglycolmonomethyl -ether	0.7-0.9 est	0.3	14 est	14 est
	LOW				
1	1,1,1,2,2,3,3-heptachloropropane (mp = 29 °C; w/heptane-20 °C; DM = 1.0) (Aldrich 25,731-1)	0.1-0.3 est	1.5	5.7 est	6.3 est
2	Pentachloroethane (DM = 0.94)	0.1-0.3 est	nd	5.7 est	6.3 est
3	1-dodecyne (DM = 0.87 est) (Aldrich 24,440-6)	0.05-0.1 est	nd	nd	nd
4	Perfluoroheptane-1H (PCR-SCM Corporation)	Low	nd	nd	nd

*nd = not determined
**est = estimate

3.3 Polarity.

Model liquids with extremely high and low polarities are listed in Table 4. The columns list quantitative measures of polarity by several scales. Low polarity as a factor is taken as a non-zero, finite polarity. Therefore, perfluoroalkanes and alkanes are not included here; however, these liquids serve as good models for other extremes in liquid state properties. Classes of liquids are listed (e.g., thioethers, thianes, disulfides, alkyl and haloalkyl ethers, and sulfides). One or more candidate liquids have been identified in each class. In general, the sulfur analogs are preferred since they are not strong HBAs. Low polarity liquids with no HB activity (e.g., haloalkanes) are also included.

Strongly polar model liquids listed are pyrrolidones, sulfoxides, nitriles, and carbonates. Aside from a few traditional solvents, several candidates with a spectrum of other solvent and physical properties are identified.

The low toxicity, higher alkyl pyrrolidones provide a range of solubility parameters, water solubilities, and vapor pressures. Partial ionic resonance structures can be rationalized, at least for N-methylpyrrolidone (NMP) (Table 4). The nitriles can be divided into monofunctional and difunctional nitriles. Glutaronitrile is the lowest MW monofunctional liquid nitrile. The dipole moment is quite high, and the ratio of bp:MW is a very high value of about three.

The bis(2-cyano)ether and thioether are also candidate model liquids with regard to their extreme polarity, high BP/MW ratio, and their family relationship to bis(2-haloethyl)ethers and sulfides. Carbonates are distinguished as having very high polarities and relatively low HBPs. In this sense, carbonates are similar to nitroalkanes. However, only the ethyl and propyl substituents are liquids at near ambient temperatures. Other liquids (e.g., DMSO, DESO, etc.), which are of special interest with respect to their rapid transport through skin, are also listed.

3.4 Density.

High and low density model liquids are listed in Table 5. The columns list their polarity, HB values, and physical properties. One class of monofunctional high density liquids is the haloalkanes, and several of these are noted.

Carbontetrabromide and/or carbontetraiodide are ideal compounds in the sense of providing high density, zero dipole moment, and finite polarizability/dipolarity; a eutectic or cosolvent system comprised of these high melting carbontetrahalides and related haloalkane liquids might be formulated as a model solvent system. Other haloalkanes of high density and moderate vapor pressure (VP) are also listed. The difunctional bromobutyronitrile and iodoacetonitrile are both of high density; but, these could also be models for high dipolarity.

The dibromothiophenes provide another difunctional class, and 3,4-dibromothiophene provides an interesting comparison to the bis(haloalkyl)sulfides and bis(cyanoalkyl)sulfides.

Table 4. Model Liquid Candidates with Extremely High and Low Polarity

Priority	Model Liquids	Dipolarity[1]	Dipole Moment debye[4]	Dielectric Constant[5]	Hansen[2]	Hoy[3]
	HIGH POLARITY					
	PYRROLIDONES					
	N-ethylpyrrolidone (NEP)					
	N-methylpyrrolidone (NMP)	0.92	4.1	32	12.3	10.4
4	Isopropylpyrrolidone (IPP)	nd	4.0 est*	nd**	nd	nd
	Cyclohexylpyrrolidone (CHP)	nd	nd	nd	nd	nd
	DICYANOALKANES AND ETHERS					
1	1, 3-dicyanopropane (K&K Laboratories #15123)	0.93	3.91	nd		nd
2	bis (2-cyanoethyl) thioether (Aldrich 5-435 17-1 $20/53)	nd	nd	nd	nd	
3	bis (2-cyanoethyl) ether	nd	nd	nd		nd
7	iodoacetonitrite (BP = 183) (1-cyano-2-iodoethane)	nd	nd	nd	nd	
	CARBONATES					
	Propylenecarbonate	0.83	4.98	66.1	3.1	nd
	SULFOXIDES					
6	DMSO	1.0	3.96	47	16.4	nd
	LOW POLARITY					
	THIOETHERS					
1	Dibutyldisulfide	0.4	2.02	nd	nd	nd
2	Dithioalkanes	nd	nd	nd	nd	13.4

*est = estimate
**nd = not determined

Table 5. Model Liquid Candidates for Extreme Values of Density

Priority	Model Liquid	Density 25 °C (g/cm^3)[5]	bp (°C)[5]
	HIGH		
	HALOALKANES		
	Carbontetraiodide (mp = 171 °C)	4.32	90-100
	eutetic with 1,3-diiodopropane	2.576	224
	Carbontetrabromide (mp = 89 °C)	3.42	190
	eutetic with 1,1,2-tribromoethane	2.579	187
	diiodomethane	3.3254	182
1	1,2,3-Tribromopropane (K&K Laboratories, #19280)	2.436	219
	1,3-diiodopropane	2.576	224
	HALO, CYANOALKANES		
	4-bromobutyronitrile	1.489	205
2	Iodoacetonitrile (Aldrich I-690-3)	2.307	183
	LOW		
1	Hexadecane	0.744	287
2	Dodecane	0.75	216.2

Low-density model liquids are represented by alkanes, and these can be identical to zero polarity, low MW model liquids.

3.5 Refractive Index (RI).

Model liquids with extreme RI values are noted in Table 6. The only low RI liquids with reasonable physical properties appear to be co-correlated with high dipolarity and high HB basicity. The properties of trimethylphosphate (TMPO), triethylphosphate (TEPO), and diethyl(sulfate) are listed, with TEPO being the liquid of choice based on its lower toxicity and an available database.

High RI model liquids consist of numerous impractical classes of solvents, such as isocyanates and fluoronaphthalenes. High RI and high density are co-correlated for many families of organics, and 3,4-bromothiophene is listed here, in addition to being listed in the density table.

Table 6. Model Liquid Candidates for Extreme Values of RI (Sodium D Line, 20 °C)

Priority		RI[5]	bp (°C)[5]
	HIGH		
	Carbondisulfide	1.6319	46
	Carbondiselenium (density = 2.7)	1.8454	126
	Diiodomethane	1.7425	182
1	3,4-dibromothiophene (Aldrich 24.715-4)	1.6395	221
	LOW		
1	Triethylphosphate	1.4045	215
	Trimethylphosphate	1.396	197
	Diethylsulfate	1.3989	208
	Perfluoroalkanes	1.29	100-253

3.6 Molecular Weight (MW).

The selection of model liquids based on extreme MW (Table 7) effects presents more of a problem than originally thought, given the advanced state of application of molar volume and cohesion parameters as reduced variables in liquid state chemistry. Fortunately, most families of liquids considered as models for extremes in MW effects are represented by a homologous series.

The approach to defining extreme liquid MW in a factorial experiment involves the following steps:

(1) Dividing the model compounds into nonpolar perfluoroalkanes and alkanes, low- or minimally-polar perfluoroglycolethers and aromatics, the moderately polar ester plasticizers, and the very polar cyanoalkanes.

(2) Selecting monodisperse molecular species and oligomers, whenever possible.

(3) Abandoning the VP criterion due to the MW-VP correlation in a series and selecting three model liquids:

(a) the lowest practical VP and, therefore, MW.

(b) the liquid at the 200 °C bp criterion.

(c) the highest MW liquid compound in a series with an mp below ambient temperature.

(4) Accepting anomalous behavior as consequence of the extreme effects studies, as discussed below.

Cyanoalkanes have relatively low MWs and VP. In the absence of HB, this degree of cohesiveness is often attributed to structure formation, such as head-to-tail dimerization. Interpretation of experimental results becomes complicated in that a low MW effect on the response variable might then be confounded by the energy of cavity formation in a low MW liquid with structure. Likewise, the perfluoroalkanes and perfluoroglycolethers provide high MW coupled with relatively low VP. An interpretation of a high MW effect might require consideration of the anomalous intermolecular repulsion effects in perfluoro compounds in addition to high molar volume effects.

These anomalous effects probably should not be avoided at this time since the full range of "normal" effects in alkanes and chloroalkanes has already been well modelled in regular solution theory.[2] Liquids with relatively high and low MWs are listed in Table 7. The values of MWs are followed by columns containing data on BP, BP/MW, density, polarity, and HBPs.

The perfluoroalkanes (Fluorinert, 3M Company) listed represent (1) the highest MW room temperature liquid, (2) a model liquid with a moderate BP of about 215 °C and an MW of 800+, and (3) a model liquid with a minimal practical BP of 101 °C (perfluoroctane). These liquids have BP/MW ratios of about 0.25.

Table 7. Model Liquid Candidates for Extreme Values of MW (g/mole)

Priority	Model Liquid	MW	bp (°C)[5]	Dipole Moment debye[4]	Dielectric Constant[5]
	HIGH				
	PERFLUOROALKANES (FLUORINERT, 3M Company)				
	FC-70 perfluorohexadecane and oligomers	820	215	0 est*	1.98
	FC-71 perfluorononadecane and oligomers	970	253	0 est	1.94
	FC-104 perfluoro-octane and oligomers	438	101	0 est	1.86
	PERFLUOROETHYLENEOXIDE (Krytox, DuPont Company) No AZ (d = 1.86 g/mL; RI 1.3)	2000	350-400	nd**	2.1-2.2
	HYDROCARBONS				
	Hexadecane	226		nd	2 est
	Nonylnaphthalene	254	369	nd	2.4-2.6 est
	DXE (1,1-di-3,-4-xylylethane) (d = 0.978 @ 60 °F; RI = 1.566) or 1,1 bis (3,4 dimethylphenyl) ethane (Aldrich 24,309-4)	238	335	0.5 est	nd
	LOW				
	Dicyanopropane (d = 0.995)	94	285	3.91	nd

*est = estimate
**nd = not determined

The perfluoroethyleneoxides (DuPont Krytox) are usually available as oligomers. Low, moderate, and high VP model liquids are selected in this series also. Weak proton acceptor capability may be present at the ether substituent.

The highest MW, ambient-temperature, liquid linear alkane (hexadecane) is also listed.

A slightly more polar set of high MW aromatics are nonylnaphthalene and DXE (Table 7). Both are important plasticizers and industrial media for reactions.

Monodisperse silicones are also of interest as model liquids, and candidates are noted at several VPs.

Extremely low MW model liquids are provided by the dicyanoalkanes. Glutaronitrile, with an MW at 94, might be an appropriate selection, although almost all of the dicyanoalkanes have BP/MW ratios of about 3.

At similar VPs (BP of about 215-285 °C), the perfluoroalkanes and dicyanoalkanes have MW ratios of about 10:1 and molar volume ratios of about 5:1. The usual range of MW or Vm ratios in solvent parameter correlations is often below 2:1.

A conceptual complexity is that the high and low polarity effects associated with MW require that the experiment be conducted to independently factor polarity effects. The experimental complexity involves the extremely low interactions of perfluoro liquids with solutes. The perfluoro liquid influence on a dependent response variable might either be below the range of measurement, or the perfluoro liquid may not dissolve a solute such that the reaction/interaction effect can be measured. Either high MW alkanes or aromatic model liquids might be required to measure a solute interaction at a significant level.

4. DISCUSSION

The model liquids selected here are most often required for bold experimental designs requiring orthogonal solvent-solute experimental data sets to minimize co-correlation. Other unusual applications can arise for which these liquid sets are useful. One application came from a request for liquids(s) that met extreme specifications for two-phase lubricating flow. This flow additive was required for a spinning, nutating liquid-filled projectile that required a high enough density relative to other fluids present to be spun to the outside projectile surface. The solvent properties were required to be different from the other fluids to ensure immiscibility. Examples of these candidates are listed in Table 8.

5. CONCLUSIONS

Over 50 liquids with extreme values of liquid state properties were identified. The properties were hydrogen bond acceptor and donor strength, polarity, refractive index, density, and molecular weight. These model liquids can be selected for investigation of solvent-solute interactions to provide bold ANOVA experimental designs, orthogonal liquid experimental sets, and minimal co-correlation amongst the experimental data.

Table 8. Candidate Two-Phase Fluid Flow Lubricants and Their Properties at 25 °C

	LIQUIDS		
	Density g/cm^3	BP °C	Viscosity, CS
REPULSIVE INTERACTIONS:			
(Oligomeric:)			
Perfluoro-nonadecane	1.96	253	73
Perfluorohexadecane	1.94	215	14
Perfluoro-octane	1.77	101	0.8
Perfluoroethyleneoxide (Various, see Table 7)	1.8 ± 0.1	300 ± 100	40-50
EXTREMELY HIGH DENSITY - DISPERSION INTERACTIONS:			
1,3-iodopropane	2.576	224	1-3 est*
1,2,3-tribromopropane	2.436	219	1-3 est
1,1,2-tribromoethane	2.579	219	1-3 est

*est = estimate

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